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## **Claims**

 A pharmaceutical composition comprising a host-rotaxane and a guest molecule in a pharmaceutically-acceptable carrier, wherein the guest molecule comprises an active agent.

- 2. The composition according to claim 1, wherein the host-rotaxane comprises at least one linear component disposed in at least one cyclic component.
- 3. The composition according to claim 1, wherein the host-rotaxane comprises at least one blocking group.
- 4. The composition according to claim 2, wherein the at least one of the blocking group comprises a linker for associating the guest molecule to the host-rotaxane.
- 5. The composition according to claim 4, wherein the linker comprises a cyclic aliphatic ethers, non-cyclic aliphatic ethers, cyclic aromatic compounds, non-cyclic aromatic compounds, anionic species, cationic species, and functionalized constructions thereof.
- 6. The composition according to claim 1, wherein the guest molecule comprises proteins, peptides, amino acids, aromatic compounds, inorganic cations, inorganic anions, organic cations, organic anions, sugars, DNA, RNA, nucleotides, phosphates, phospholipids, fatty acids, steroids, isoprene derivatives.
- 7. The composition according to claim 2, wherein the host-rotaxane further comprises at least one recognition element.
- 8. The composition according to claim 7, wherein the at least one recognition element is attached to at least one cyclic component.
- 9. The composition according to claim 3, wherein the at least one recognition element is capable of forming an interaction with the linker, the guest molecule or a combination thereof.
- 10. The composition according to claim 9, wherein the interaction comprises hydrogen bonds, electrostatic interactions, dispersion interactions or a combination thereof.

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11. The composition according to claim 7, wherein the at least one recognition element comprises carboxylates, ammonium ions, guanidinium ions, imidazolium ions, phosphates, aromatic rings, aliphatic groups, alcohols, amides, carboxylates, sulfhydryls, or combinations thereof.

- 12. The composition according to claim 4, wherein the host-rotaxane comprises at least one polar recognition element on at least one cyclic component.
- 13. The composition according to claim 1, wherein the agent is a therapeutic agent.
- 14. The composition according to claim 1, wherein the composition further comprises a binding element.
- 15. The composition according to claim 14, wherein the binding element comprises a marking element.
- 16. The composition according to claim 15, wherein the marking element is a fluorophore.
- 17. A composition comprising a host-rotaxane and an agent.
- 18. The composition according to claim 17, wherein the agent comprises a vaccine, a drug, a prodrug, or a derivative or an analog thereof.
- 19. A method of delivering an agent to a subject, comprising administering to the subject a composition comprising a host-rotaxane and an agent.
- 20. The method according to claim 19, wherein the agent is administered prior to, concurrently, or subsequently to the administration of the host-rotaxane.
- 21. The method according to claim 19, wherein the agent comprises a vaccine, a drug, a prodrug, or a derivative or an analog thereof.
- 22. The method according to claim 19, wherein the agent is administered to target cancers, tumors, malignancies, uncontrolled tissue, cellular proliferation, or a combination thereof.
- 23. The method according to claim 19, wherein the composition is administered orally, parenterally, intrasystemically, intraperitoneally, topically or combinations thereof.

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24. The method according to claim 19, wherein the composition comprises a pharmaceutically acceptable carrier.

- 25. The method according to claim 14, wherein the carrier comprises a solid, semisolid, liquid filler, diluent, or encapsulating material.
- 26. The method according to claim 19, further comprising a subsequent administration of an agent to the individual.
- 27. The method according to claim 20, further comprising a subsequent administration to the individual of a guest molecule bound with an agent.
- 28. A method of treating cancerous cells in an individual, comprising administering to the individual a composition comprising a host-rotaxane, a guest molecule and an agent bound to the host-rotaxane, wherein the composition delivers the agent to the cancerous cells.
- 29. The method according to claim 28, wherein the cancerous cells are a tumor.
- 30. The method according to claim 28, wherein the agent is a drug, a prodrug, or a derivative or an analog thereof.
- 31. A method for diagnosing cancerous cells in an individual, comprising administering to the individual a composition comprising a host-rotaxane, a guest molecule and a marking element and diagnosing the cancerous cells in the individual.
- 32. The method according to claim 31, wherein the marking element comprises a fluorophore.
- 33. The method according to claim 31, wherein the cancerous cells are diagnosed by imaging.
- 34. The method according to claim 19, wherein the host-rotaxane is conjugated to a target-binding moiety.